User manual

Toolbox 4.3 Release Notes

Document history

Version	Comment
Version 1.0	January 2019: Toolbox 4.3 Release Notes

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If you have questions or comments that relate to this document, please send them to ehscont@oecd.org or visit the QSAR Toolbox discussion forum at https://community.oecd.org/community/toolbox_forum

Table of Contents

1 Overview

The Toolbox 4.3 installation is a major update of Toolbox 4.2. It can be installed as a separate product alongside previous major releases of Toolbox (4.2, 4.1, 4.0, 3.4, 3.3, etc.)

2 System Requirements

Minimum system requirements

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OS: 64 bit, Windows 7 or newer

CPU: Core 2 duo at 2 GHz or equivalent AMD CPU

RAM: At least 4GB of RAM

HDD: 14 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

Recommended system requirements

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OS: 64 bit, Windows 7 or newer

CPU: I5 at 2.4GHz or faster processor or equivalent AMD CPU

RAM: 6 GB of RAM

HDD: 20 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

3 Change log

I. New additions

1. **Databases: 2 new databases** (*pKa OASIS*, *ADME database*)
2. **Profilers*:* 5 new profilers** (*Acute Oral Toxicity*, *Blood brain barrier (beta)*, *Oral absorption (beta)*, *Skin permeability (beta)*, *Uncouplers (MITOTOX)*)
3. **2D parameters: 5 new methods for assessing pKa**
4. (**Q)SAR models: 159 new (Q)SAR models** – including pre-calculated online Danish QSAR DB models and new pKa models
5. **New functionalities:**
   - **(Q)SAR editor** – possibility to create custom (Q)SAR model by dynamic link to external online QSAR computational platform or by equation; possibility to edit, import and export the custom profilers
   - **Effectopedia Wizard** – connection between Toolbox and Effectopedia is possible now
   - **Stereo information** - New buttons for drawing stereo bonds in the 2D editor and visualization of the stereo information on the data matrix
   - **ChemID –** possibility to search by additional chemical identifier (EC number); possibility to include additional ID information in the custom inventories during the import
   - **Public API -** Toolbox application program interface is now publicly available. This allows software developers to enrich Toolbox tools library with additional parameter calculators, profilers, (Q)SAR models and metabolism simulators.

II. Improvements

1. **Updated databases: 5 updated databases**
   - ***ECHA CHEM*** *(dissemination November 2018)* - 11 735 chemicals with 668 041 data are available now
     - corresponding to IUCLID 6.2

- Endpoints with the most new experimental data: *aquatic toxicity* (3 205 chemicals and 46 347 data points), *irritation/corrosion* (3 549 chemicals and 120 121 data points), *sensitization* (2 101 chemicals and 6 614 data points)

- ***ECOTOX*** *(September 2018)*– 11 655 chemicals with 917 046 data are available now
  - 335 chemicals and 29 931 data points are new
- **Genotoxicity OASIS** – 7985 chemicals with 30 447 data are available now
  - 55 chemicals and 507 data points are new
- **Hydrolysis rate constant OASIS** – 349 chemicals with 349 data are available now
  - 8 chemicals and 8 data points are new
- **Repeated Dose Toxicity HESS** – new metadata are included

2. Updated profilers and simulators

- 16 updated profilers
- 7 updated metabolism simulators

3. Improved functionalities

- Showing the database affiliation of the results when search for a chemical by CAS/Name/SMILES
- Removing of the duplicated SMILES when load a list with SMILES
- "Alert performance" (AP) functionality – selection of an alert for primary grouping directly from the *Alert performance results* window is possible now
- Reorganization of the report wizard pages in order to improve the user-friendliness of the reports
- Possibility to manage the report basket items (to rearrange (move up/down), to rename or to delete)

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